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PROCEEDINGS OF THE EPA WORKSHOP ON THE ENVIRONMENTAL SCORING OF CHEMICALS

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CONTENTS

Figures v
Tables vii
Preface ix
Abstract xi
1. Introduction 1
2. San Antonio Environmental Subgroup Summary 4
3. Integration of Scoring Systems of Environmental Subgroups . . . 4
4. Testing and Modification of the Integrated System 19
5. Testing the Modified Scoring System 30
6. Discussion and Conclusions 30
Appendix 36
References 37

FIGURES

1. Toxicity matrix for proposed scoring system 5

2. Data needed for estimation of environmental concentrations . . 25

TABLES

1. Chemicals used to test scoring system 3

2. Scoring system for environmental toxicity 6

3. Scoring system for bioaccumulation in aquatic species 7

4. Scoring system for persistence, bioaccumulation potential, and mobility 8

5. Scoring system for environmental concentration 9

6. Ecosystem components of scoring system 10

7. Format for displaying exposure and fate of chemicals 12

8. Format for displaying effects 13

9. Format for displaying hazard evaluation 15

10. Comparison of separate scoring exercises 20

11. Revised format for displaying effects 22

12. Revised format for displaying hazard evaluation 23

13. Format for displaying environmental exposure 26

14. Phase-one scoring format for displaying effects 27

15. Toxicity multipliers of environmental exposure scores 29

16. Toxicity multipliers determined by scoring of test chemicals 31

17. Environmental exposure scores of test chemicals 32

18. Integration of toxicity multipliers with environmental exposure scores 33

PREFACE

This report is a product of the Health and Environmental Studies Program (HESP) of the Information Center Complex (ICC), Information Division, Oak Ridge National Laboratory (ORNL). It was prepared for the Assessment Division, Office of Toxic Substances, U.S. Environmental Protection Agency (EPA).

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ABSTRACT

The environmental scoring of chemicals is viewed by the U.S. Environmental Protection Agency as a tool to assist in the ranking or ordering of the universe of chemicals that are under the jurisdiction of the Toxic Substances Control Act. The purpose of scoring is to identify most of the chemicals that have a high probability for requiring review for regulation or testing. This report describes a three-day workshop held in Washington, D.C., August 13-15, 1979, to develop an environmental scoring system. Initial discussions centered on the determination of a safety factor (calculated as the concentration at which an effect is observed divided by environmental concentration) that would allow a numerical score to be assigned to a chemical to reflect its potential hazard. Further discussion, however, indicated that the environmental concentration of a chemical is usually not available and that the estimation of an environmental concentration is not readily accomplished; therefore, a scoring system was developed that does not require environmental concentrations. This system relates environmental exposure to toxicity by using a multiplier (3×, 2×, or 1×) which is assigned on the basis of the concentration at which an effect is observed. The applicability of the scoring system is demonstrated by scoring selected chemicals.

1. INTRODUCTION

The Toxic Substances Control Act (TSCA) mandates the U.S. Environmental Protection Agency (EPA) to control substances that are harmful to human health or the environment. In addition, it enables the agency to require testing on existing poorly characterized chemicals that may present unreasonable risks to human health or the environment or that have significant production volume, human exposure, or environmental release. The Interagency Testing Committee (ITC) was established by TSCA and instructed to recommend to EPA a list of priority chemicals that should be considered for testing.

The EPA and ITC require a system to assist them in ranking or ordering the universe of TSCA chemicals so that chemicals with the greatest need for control and testing are identified and reviewed first. Scoring is viewed as a tool to assist in the ordering at an early stage in the assessment process. As such, scoring serves to identify chemicals that should receive additional scientific review; it should not be used to make ultimate regulatory decisions.

Because scoring is a screening tool, it assumes some compromise between completeness and speed. The accuracy of the ranking depends on having a complete data base, yet investment of elaborate resources in this area defeats its purpose as a screen. The necessary simplicity of scoring acknowledges that some chemicals will slip through the screen, and additional scientific judgment is needed to add those problem chemicals that the scoring system could not accommodate. The purpose of scoring is to identify most of the chemicals that have a high probability of requiring review for regulation or testing.

The Assessment Division of EPA is that part of the Office of Toxic Substances responsible for the first phases of evaluating chemicals under TSCA, including their selection. It shares ITC's need for a system to rank TSCA chemicals requiring testing, but the system used by the Assessment Division should also select chemicals possibly needing control. To some extent the current ITC system, which uses positive scores to denote documented hazards and negative scores to denote suspected hazards, can accommodate both goals.

Shortly after it was formed ITC developed a scoring system to rank chemicals in order of their need for testing (Federal Register, 1977). Chemicals from a variety of source lists received exposure scores and biological effects scores that covered seven subfactors dealing with human health and ecological concerns. Recognizing a need for an evaluation of the system, ITC conducted a workshop in February 1979 in San Antonio, Texas, to examine the scoring method of each of the subfactors, to assess the means used for weighing and combining the scores, and to recommend revisions, if needed.

The environmental scoring system that took shape at the February 1979 ITC workshop consisted of three segments: environmental (biotic) effects, environmental fate, and ecosystem effects. Due to lack of time in February, certain elements of the scoring system were not completed, and the three segments were not integrated.

Sharing a common need to examine the environmental scoring system and similar logic and information needs in this area, the Assessment Division and ITC cooperated to complete the environmental effects scoring system. The Assessment Division with the support of ITC sponsored a workshop August 13-15, 1979 to integrate the components developed at the ITC February 1979 workshop and to test the scoring system on several chemicals (listed in Table 1). The Health and Environmental Studies Program of the Oak Ridge National Laboratory, through an interagency agreement, arranged the workshop and supplied dossiers on the chemicals in Table 1 for use by workshop participants (see Appendix). Information in the dossiers was the primary data source for the scoring exercises.

This report of the proceedings of the August 1979 workshop includes an explanation of the scoring system and how it might be used by those persons responsible for developing a priority ranking of chemicals needing further assessment for possible testing or control. To understand the full development of the system, the reader is directed to the original ITC scoring system (Federal Register, 1977) and the report from the ITC workshop held in February 1979 (TSCA-ITC Workshop, 1979).

Two major points stressed by participants throughout the workshop were the necessity of having at least a minimal amount of data on a chemical before scoring could occur and the necessity that a scoring

Table 1. Chemicals used to test scoring system

Ammonia
Chlordane
Diethyl hexylphthalate
Hexachlorocyclopentadiene
Leptophos
Linear alkyl sulfonate
Nitrilotriacetic acid
Quinaldine
Tetraethyllead
2,4-Xylenol

system be relatively simple. The evolution of the scoring system as described in this report reflects these two concerns.

2. SAN ANTONIO ENVIRONMENTAL SUBGROUP SUMMARY

At the San Antonio Workshop in February 1979, the environmental subgroups on toxicology (E_1) and fate and chemistry (E_2) developed separate scoring systems, and the third environmental subgroup (E_3) identified areas of consideration for scoring ecosystem effects. (This third subgroup concluded its task at a June 13, 1979 meeting in Washington, D.C.) Figure 1 shows the E_1 matrix which, when completed using the criteria for scoring environmental toxicity in Table 2 and the criteria for scoring bioaccumulation in Table 3, permits a hazard value to be derived by totaling the numbers in the matrix. In many cases both negative and positive numbers will appear in the table and should be added separately to give a negative total and a positive total. The negative number indicates that data exist which suggest a possible hazard, whereas the positive number indicates a documented hazard.

Tables 4 and 5 show the scoring system criteria selected by the fate and chemistry subgroup. Final scores are reached by adding the negative (suspected hazards) and positive (documented hazards) scores separately. It should be noted that both the toxicology subgroup and the fate and chemistry subgroup used the parameter of bioaccumulation, and both also require either estimated or measured environmental concentrations to arrive at a final score. (Subgroup E_1 used estimated concentrations; subgroup E_2 used measured concentrations.)

Areas of consideration identified by the ecosystem effects subgroup (E_3) are given in Table 6. The scoring rules for these parameters are too detailed for complete presentation in this report but can be found in the reported proceedings of the San Antonio Workshop (TSCA-ITC Workshop, 1979).

3. INTEGRATION OF SCORING SYSTEMS OF ENVIRONMENTAL SUBGROUPS

The charge for the first day of the August 1979 workshop was to integrate the individual scoring systems developed by the three subgroups

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	MICROBES, ALGAE, PLANTS	INVERTEBRATES	FISH	BIRDS, MAMMALS
LETHALITY				
GROWTH/DEVELOPMENT				
REPRODUCTION				
BIOACCUMULATION				
OTHER TOXICOLOGICAL EFFECTS				

Fig. 1. Toxicity matrix for proposed scoring system.

Table 2. Scoring system for environmental toxicity[a]

Score	Criterion
+3[b]	Known EC_{50} less than the EEC[c]
+2	Known EC_{50} between the EEC and 10 times the EEC
+1	Known EC_{50} between 10 and 100 times the EEC
0	Known EC_{50} greater than 100 times the EEC
-1	Estimated[d] EC_{50} greater than 10 times the EEC
-2	Estimated EC_{50} between 1 and 10 times the EEC
-3	Estimated EC_{50} less than the EEC

[a]Does not include bioaccumulation, which is given in Table 3.

[b]The numerals designating the scores are not an arithmetical series of integers: +3 and -3 both designate levels of greatest effect.

[c]EEC = estimated environmental concentration.

[d]Estimated values will be based on structure/activity relationships or data on related organisms.

Source: TSCA-ITC Workshop, 1979, Table 1, p. 48.

Table 3. Scoring system for bioaccumulation in aquatic species

Score	Criterion
+3	Measured BCF[a] greater than 10,000
+2	Measured BCF between 1,000 and 10,000
+1	Measured BCF between 100 and 1,000
0	Estimated[b] BCF less than 100
-1	Estimated BCF between 100 and 1,000
-2	Estimated BCF between 1,000 and 10,000
-3	Estimated BCF greater than 10,000

[a]BCF = bioconcentration factor, which is the concentration in tissue or animal divided by the concentration in water.

[b]Estimate based on the *n*-octanol/water partition coefficient.

Source: TSCA-ITC Workshop, 1979, Table 2, p. 48.

Table 4. Scoring system for persistence, bioaccumulation potential, and mobility

Score	Persistence	Bioaccumulation potential[a]	Mobility
+3	Infinite	High	High
+2	Up to 1 year	Appreciable	Medium
+1	1 to 8 weeks	Low	Low
0	Up to 1 week	Negligible	Negligible
-1	Suspected low; no data	Suspected low; no data	Suspected low; no data
-2	Suspected high; no data	Suspected high; no data	Suspected high; no data

[a]Based on the *n*-octanol/water partition coefficient.

Source: TSCA-ITC Workshop, 1979, Table 4, p. 60.

Table 5. Scoring system for environmental concentration

Score	Environmental Concentration		
	Soil	Water	Air
+3	10 ppm	1 ppm	1,000 ng/m^3
+2	1 to 10 ppm	0.1 to 1 ppm	100 to 1,000 ng/m^3
+1	0.1 to 1 ppm	0.01 to 0.1 ppm	10 to 100 ng/m^3
0	<0.1 ppm	<0.01 ppm	<10 ng/m^3
-1	Suspected low; no data	Suspected low; no data	Suspected low; no data
-2	Suspected high; no data	Suspected high; no data	Suspected high; no data

Source: TSCA-ITC Workshop, 1979, Table 5, p. 60.

Table 6. Ecosystem components of scoring system

Primary production
Secondary production
Population changes
Nutrient cycles
Ecosystem structure and function
Diversity/simplicity
Endangered species and habitat

Source: Adapted from TSCA-ITC Workshop, 1979, Figure 1, p. 65.

(E_1, E_2, and E_3) so that areas of overlap and omissions were resolved and the three operated well together. This integrated or combined scoring system could be used to develop a priority ranking of chemicals; the chemicals receiving high scores in the ranking were those that would receive additional review to determine what, if any, testing or control is necessary.

By the close of the first day's session, an integrated system was developed that the participants considered a starting point for assessing the chemicals listed in Table 1, realizing, however, that modifications would be made as a result of tests of the scoring system performed during the workshop. Tables 7, 8, and 9 show the components of the integrated system. The table for displaying exposure and fate (Table 7) is somewhat similar to Tables 4 and 5, which were developed at the San Antonio Workshop, in that all three tables consider essentially the same parameters of release rate, redistribution potential, and degradation. The release rate can be defined as the combined amount of a chemical released to a given medium (note in Table 7 the exclusion of sediment and biota; chemicals enter these compartments either through the soil, air, or water) from manufacture, use, and disposal. The values for release rates are expressed in lbs/yr and are entered for the appropriate medium in Table 7.

The redistribution potential indicates the likelihood that a chemical that has entered the environment through one medium (air, water, or soil) will be distributed to one or both of the other two or to the sediment and biota. As indicated in Table 7, the redistribution potential in any compartment is primarily a function of its physical properties. The important parameters that determine the redistribution of a chemical in the environment are the air/water distribution coefficient, the water/soil distribution coefficient, and the water/biota distribution coefficient.

The air/water distribution coefficient (H_c) may be determined either by direct measurement,

$$H_c = \frac{\text{concentration in air (mg/liter)}}{\text{concentration in water (mg/liter)}} ,$$

Table 7. Format for displaying exposure and fate of chemicals

	Soil	Air	Water	Sediment	Biota
Release rate					
Redistribution potential	[a]	[b]	[a], [e]	[a]	[e] [f]
Degradation					
Estimated concentration					
Measured concentration					

[a] Soil adsorption coefficient/% carbon.
[b] Vapor pressure.
[c] Henry's constant.
[d] Solubility.
[e] Bioconcentration factor.
[f] Partition coefficient.

Table 8. Format for displaying effects

	Abiotic	Bacteria	Plants	Invertebrates	Fish and other aquatic vertebrates	Birds and mammals	Simulated ecosystems	Field ecosystems
Short term								
Long term								
Lethality								
Growth and development								
Reproduction								
Pathology								
Ecosystem processes								
Primary production								
Secondary production								
Population changes								
Nutrient cycles								
Ecosystem structure and function								
Diversity/simplicity								
Endangered species and habitat								

Table 8 (continued)

	Abiotic	Bacteria	Plants	Invertebrates	Fish and other aquatic vertebrates	Birds and mammals	Simulated ecosystems	Field ecosystems
Other toxic effects								
Behavioral								
Physiological								
Meteorological								

[i]Genetic defects induction and reproductive success.

[j]Results of gross and microscopic pathology of organ systems including functional, structural, or size abnormalities and benign or carcinogenic tumor induction.

[k]Ecosystem effects include effects on:

Primary productivity - assessed by direct and indirect measurements (standing crop, dry weight yield, chlorophyll, CO_2 fixation rate) and remote sensing (light absorbance);

Secondary productivity - growth and development - reflecting material transformation as assessed by direct and indirect measurements (standing crop, photosynthesis/respiration ratios, etc.);

Nutrient cycling and material sequestering - decomposition - assessed by direct and indirect measurements (litter crop changes, community respiration, nutrient losses);

Population dynamics - reproduction assessed by direct measurements of age-class distributions, recruitment rate, fecundity, etc. and laboratory measurements on developmental phenomena for individual species;

Ecosystem structure and function - assessed by examination of key species and processes in the laboratory and field (This may involve elements of all or parts of the first four ecosystem effects components);

Ecosystem diversity/simplicity - assessed by a number of indices of diversity of richness by species enumeration/mass; and

Endangered species and their habitats - specialized assessments of all of the above ecosystem effects components, but considered significant enough to arouse, independently, ecological concern (TSCA-ITC Workshop, 1979).

Table 9. Format for displaying hazard evaluation

	Abiotic		Bacteria	Plants		Invertebrates		Fish and other aquatic vertebrates	Birds and mammals	Simulated ecosystems		Field ecosystems	
	T[a]	A[b]	A	T	A	T	A	A	T	T	A	T	A
Short term													
Long term													
Other effects													

[a] Terrestrial.
[b] Aquatic.

or by appropriate treatment (see MacKay, Shiu, and Sutherland, 1979) of vapor pressure and water solubility data with special attention to the applicability of Henry's law and Raoult's law.

The water/soil distribution coefficient can be either measured directly or estimated from information on water solubility or the octanol/water partition coefficient. For organic compounds a good correlation has been found empirically to exist between the octanol/water partition coefficient (K_{ow}) and K_{oc}, where

$$K_{oc} = \frac{K_d}{\%\ \text{organic carbon in soil}} \times 100$$

(Karickhoff, Brown, and Scott, 1979) and K_d is the measured soil adsorption coefficient:

$$K_d = \frac{\text{mg chemical/kg soil}}{\text{mg chemical/liter water}} .$$

Since there is a good correlation between K_{ow} and K_{oc} (0.98 for the organic compounds studied by Karickhoff and coworkers), reasonable estimates of K_{oc} can be made from K_{ow} if the calculations for K_{oc} cannot be performed (Karickhoff, Brown, and Scott, 1979).

The water/biota distribution coefficient (bioconcentration factor, or BCF) can be measured directly or estimated with the use of appropriate regression equations from water solubility or the octanol/water partition coefficient (K_{ow}). The appropriate regression equations are:

$$\log \text{BCF} = 0.76 \log K_{ow} - 0.23$$

for aquatic organisms that contain approximately 8% lipids (Veith et al., cited by Federal Register, 1979) and

$$\log K_{ow} = 5.00 - (0.670 \log S) ,$$

where S is aqueous solubility in μmol/liter (Chiou et al., 1977).

Chemicals released to the environment will accumulate somewhere unless they degrade and lose their chemical identity. Degradation routes are highly specific for each chemical, but certain generalizations can be made in terms of media:

1. Air

For organic chemicals, atmospheric degradation may depend on direct photolysis (adsorption of light followed by decomposition) or secondary reactions (attack by reactive atmospheric components: OH radical, ozone, oxygen atoms, etc.). Of these, degradation by OH radical attack appears to be the most prevalent (Pitts et al., 1978). Attack by OH can be measured directly in the laboratory or estimated by structure/activity relationships. In general, any organic molecule with C-H bonds or C=C bonds will be subject to degradation by OH radical attack (hydrogen subtraction or addition to the double bond). Alternatively, the photodegradation of chemicals can be studied in smog chamber type studies using artificial light. In any event, the desired outcome is an estimation of the lifetime of the chemical in the atmospheric environment, expressed in terms of half-life, $t_{1/2}$.

2. Water

Chemicals may degrade in water via a variety of mechanisms, the most prevalent of which are hydrolysis and biodegradation. Aqueous photodegradation is also important for some chemicals. A variety of measurement techniques are used to obtain an estimation of the lifetime of a chemical in water, expressed as $t_{1/2}$. It is to be noted that removal from water by other mechanisms (such as volatilization, adsorption, and bioaccumulation) was considered as redistribution.

3. Soil

Degradation of organic compounds in soil is usually via biodegradation. Direct measurement techniques, often involving ^{14}C-labeled compounds, may be used. Further, biodegradation rates in aqueous systems

are often used as estimates of degradation rates in soil. The desired output is an expression of the lifetime of a chemical in soil. Mobility of the chemical in soils, e.g., soil adsorption, is considered in the discussion of redistribution potential.

The principal reason for inclusion of data on release rate, redistribution potential, and degradation potential in Table 7 is to estimate environmental concentrations. Two approaches to estimating environmental concentrations are mathematical modeling and benchmark chemicals. With each approach, the data on release rate, redistribution potential, and degradation are used, but in somewhat different ways. The mathematical model fits existing data to the equations and derives the environmental concentration. The benchmark chemical approach, however, compares existing data on the environmental parameters of a chemical under study with a reference chemical whose environmental parameters and concentrations are known; such comparisons allow estimates of concentration based on the similarity of the environmental parameters of the chemical under consideration and the reference (benchmark) chemical. A more powerful approach is to combine the mathematical model and the benchmark chemical method. The mathematical model is used to predict the environmental concentrations of both the benchmark chemical and the chemical under study. Output from the model then allows a more realistic extrapolation of the environmental concentration of the benchmark chemical to the concentration expected for the new compound. If a measured concentration is known, however, there is no need for an estimation. Importance is placed on the environmental (exposure) concentration because it is the denominator in the equation used to assign scores to biotic effects:

$$\frac{\text{lowest effect concentration}}{\text{exposure concentration}} = \text{safety factor.}$$

The lowest effect concentration (i.e., lowest concentration in which an effect is observed) is entered into Table 8. This table is essentially a compilation of Fig. 1 (toxicity matrix) and Table 6 (ecosystem processes) with the addition of the abiotic column. Upon completion of Table 7 the exposure concentration is available.

After Tables 7 and 8 are completed, the safety factor is determined, as indicated in the above equation, by dividing the lowest effect concentration by the appropriate estimated or measured exposure concentration (e.g., effect concentration in fish is divided by concentration in water). This value is compared with the scoring criteria in Table 3 to obtain a numerical value, which is placed appropriately in Table 9 to show hazard evaluation. If more than one exposure concentration is available for a given medium, then the choice of which one to use as the denominator in calculating the safety factor depends on whether the worst case or best case is to be reflected. The lower the exposure concentration, the greater the safety factor, and the greater the exposure concentration, the lower the safety factor. After Table 9 is completed, the scores can be totaled and compared with other chemical hazard evaluation scores for priority ranking. It should be emphasized that the information entered into Tables 7 and 8 is raw data and values entered into Table 9 are numerical data based on comparisons of the safety factor with the criteria in Table 3.

4. TESTING AND MODIFICATION OF THE INTEGRATED SYSTEM

On the second day of the conference, the participants met to identify problems in the use of the integrated system (Tables 7, 8, and 9) and to determine the consistency of the scores from two independent groups. Participants were divided into two groups, each having access to basically the same information (chemical dossiers), and asked to score the same four compounds (leptophos, chlordane, diethylhexylphthalate, and nitrilotriacetic acid) using the scoring system as presented in Tables 7, 8, and 9.

After both groups had scored the compounds, they reconvened and compared their scores (Table 10). It was soon evident that discrepancies existed, especially with the scores for chlordane and leptophos. During the ensuing discussion several reasons for these discrepancies became clear. Group one had added bioaccumulation to Table 9 and, when a bioaccumulation factor was reported, compared it with the range of values in Table 3 to obtain a value for Table 9; group two did not use bioaccumulation. Another discrepancy was that group one did not use negative numbers

Table 10. Comparison of separate scoring exercises

	Group 1	Group 2
Chlordane	+19, -6	+12, -8
Leptophos	+8	0, -24
Nitrilotriacetic acid	0	0, -1
Diethyl hexylphthalate	+8, -3	+8, -6

(representing estimated or suspected hazards) to the extent that group two did; instead, group one left most of the entries blank when there were insufficient data. After some discussion, the scoring system was adapted as follows to resolve these discrepancies.

1. Bioaccumulation was included on the hazard evaluation matrix.
2. Simulated ecosystem data were omitted from the hazard evaluation matrix because of the difficulty of interpretation of data and the inability to incorporate these data into the ecosystem component as indicators or predictors.
3. The birds and mammals category was split so that bird data and mammal data could be considered separately. This facilitates the use of mammal data generated for human health effects evaluation.
4. The lowest "no effect" value was used to derive the hazard evaluation score in each long-term component (Tables 8 and 9). Where "no effect" information is absent and for short-term effects, the lowest concentration producing an effect should be used.
5. The subheadings under ecosystem processes were omitted. They were not used during the scoring exercises because there were no available data.
6. For given environmental exposure concentrations, the use of the lowest detected value will result in the largest (least conservative) safety factor, whereas the use of the greatest detected value will result in the smallest (most conservative) safety factor.
7. In categories where effect and "no effect" data are absent, no score should be assigned. A score should be assigned only when the data exist or can be extrapolated from another category or a similar chemical.

As a result of the changes noted in points 1, 2, 3, and 5, Tables 8 and 9 were modified as shown in Tables 11 and 12, respectively. The second day closed with a brief discussion that emphasized the importance of the estimated environmental concentration since most chemicals do not have adequate monitoring data and therefore no measured environmental concentrations.

Table 11. Revised format for displaying effects

	Abiotic and other	Fungi and bacteria	Plants	Invertebrates	Fish and other aquatic vertebrates	Birds	Mammals	Ecosystems
Short term								
Long term Lethality								
Growth and development								
Reproduction								
Pathology								
Ecosystems processes								
Other toxic effects Behavioral								
Physiological								
Meteorological								

Table 12. Revised format for displaying hazard evaluation

	Abiotic		Bacteria	Plants		Invertebrates		Fish and other aquatic vertebrates	Birds	Mammals		Ecosystems	
	T[a]	A[b]	A	T	A	T	A	A	T	T	A	T	A
Short term													
Long term													
Bioaccumulation	X	X											
Other	X	X											

[a] Terrestrial.
[b] Aquatic.

The final day of the workshop began with a continuation of the previous afternoon's discussion concerning the estimation of the environmental concentration. A presentation was given which outlined the parameters involved in predicting an environmental concentration (Fig. 2) and demonstrated the complexity of making such predictions; for many chemicals much of the needed information is unavailable and at present not easily estimated.

After this presentation and a reminder that the proposed scoring system was to serve as a screen and not as a substitute for risk assessments, the requirement of having the environmental concentration was eliminated. It was agreed that using measured or estimated environmental concentrations was highly desirable but such a constraint would drastically limit the number of chemicals that could be screened. Efforts were then made to design a scoring system that could make use of exposure indicators without requiring estimated or measured concentrations. Consequently, a major modification occurred in the existing scoring system as it appears in Tables 7, 11, and 12. Table 7 was altered to the Table 13 format, with the most significant change being the omission of environmental concentrations. At one point the mobility and persistence scores in Table 13 were additive; however, trial chemical scoring indicated that in some cases the spread in scores between two compounds whose mobility and persistence were greatly different was not as significant as when the scores were multiplied. For example, compound A has a mobility score of 2 and a persistence score of 2, and compound B has a mobility score of 4 and a persistence score of 4; by addition, compound A has a combined mobility and persistence score of 4 and compound B a score of 8, whereas by multiplying the scores, compound A still has a score of 4 but compound B has a score of 16. The workshop participants decided that the increased range of scores obtained by multiplying persistence and mobility scores was preferable.

Since simplicity was one of the desired attributes of the scoring system, the essential categories from Table 11 were condensed, as shown in Table 14. With the elimination of the requirement for environmental concentrations, the safety factor (calculated as the effect concentration divided by the environmental concentration) could not be used; therefore,

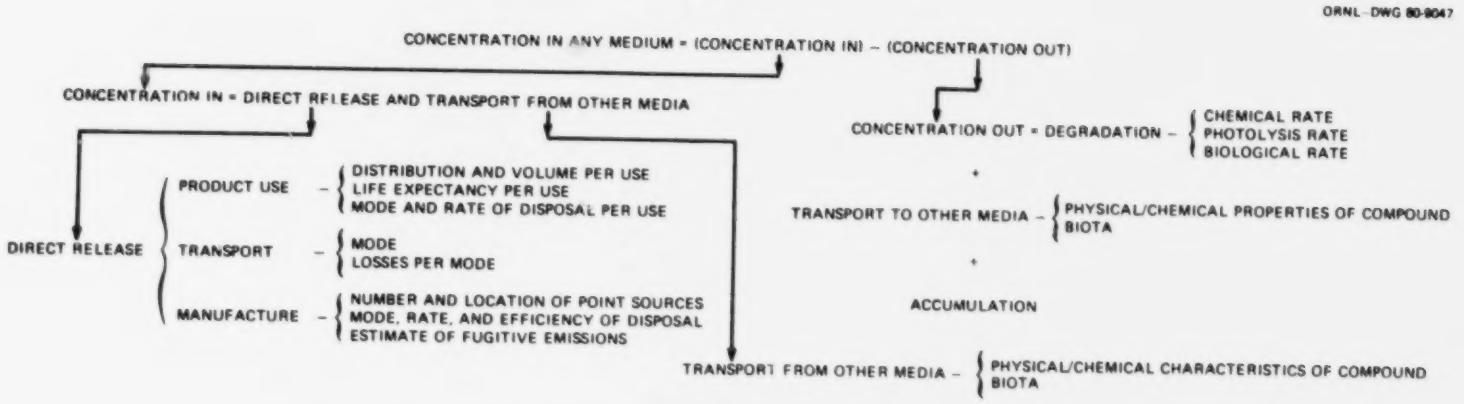
ORNL-DWG 80-9047
CONCENTRATION IN ANY MEDIUM = (CONCENTRATION IN) – (CONCENTRATION OUT)
CONCENTRATION IN = DIRECT RELEASE AND TRANSPORT FROM OTHER MEDIA
CONCENTRATION OUT = DEGRADATION – CHEMICAL RATE, PHOTOLYSIS RATE, BIOLOGICAL RATE
+
TRANSPORT TO OTHER MEDIA – PHYSICAL/CHEMICAL PROPERTIES OF COMPOUND, BIOTA
+
ACCUMULATION
DIRECT RELEASE
PRODUCT USE – DISTRIBUTION AND VOLUME PER USE, LIFE EXPECTANCY PER USE, MODE AND RATE OF DISPOSAL PER USE
TRANSPORT – MODE, LOSSES PER MODE
MANUFACTURE – NUMBER AND LOCATION OF POINT SOURCES, MODE, RATE, AND EFFICIENCY OF DISPOSAL, ESTIMATE OF FUGITIVE EMISSIONS
TRANSPORT FROM OTHER MEDIA – PHYSICAL/CHEMICAL CHARACTERISTICS OF COMPOUND, BIOTA

Fig. 2. Data needed for estimation of environmental concentrations.

Table 13. Format for displaying environmental exposure

Release volume (lbs/year)	10^8	10^6	10^4	
Score	3[a]	2	1	=
Release distribution	Global	National	Local	
Score	3	2	1	=
	Mobility[b] score		Persistence[b] score	
Soil		×		=
Air		×		=
Water		×		=
Bioaccumulation[c]	P >10^5	P = 500-10^5	P = 1-500	P <1
Score	4	3	2	1 =
			Total score	=

[a]Numbers are potential points for subfactors of the environmental exposure score. The number may be positive (indicating documented data) or negative (indicating suspected data). However, values are added as absolutes.

[b]Scored on a scale of 1 to 4. For mobility 4 = easily dispersed among three media, 3 = easily dispersed between two media, 2 = easily dispersed through one medium, and 1 = negligible dispersal. For persistence 4 = infinite, 3 = up to 1 yr, 2 = 1 to 8 wk, and 1 = up to 1 wk. Scores may be negative, indicating suspected mobility or persistence; however, values are multiplied as absolutes.

[c]P represents the octanol/water partition coefficient.

Table 14. Phase-one scoring format for displaying effects[a]

Chemical	Terrestrial species				Aquatic species				
	Plants	Birds	Mammals	Mean	Microbes	Plants	Invertebrates	Fish	Mean
Acute	[b]								
Chronic									

[a]Phase one identifies chemicals needing further review in contrast to phase two, which identifies environmental hazards that are associated with a chemical and as such require environmental concentrations to establish the degree of hazard.

[b]Toxicity multiplier from Table 15 is placed in appropriate box.

the hazard evaluation table (Table 12), which depended upon the safety factor for its values, was also eliminated. Also pertinent to the elimination of Table 12 is the fact that a hazard evaluation of a chemical is really not necessary for this first phase, or initial ranking of chemicals for further review. From this point on, the scoring system was viewed as having two phases; the first phase would consist of a priority ranking of chemicals to be considered for further review and as such would not require environmental concentrations. Phase two would be a hazard evaluation of the highest priority chemicals as identified in phase one and would require environmental concentrations.

Since the use of the safety factor was not needed for this first phase, a new way to relate environmental exposure and toxicity had to be developed. After some discussion a set of threshold levels of concern was developed (Table 15) that could be used to complete Table 14 and as multipliers (3×, 2×, or 1×) of the environmental exposure scores from Table 13. When using the information in Table 15 one should use the lowest effect concentration from a given set of raw data on the toxic effects of a compound if the greatest potential toxicity of a chemical is to be represented. This is because the lower the effect concentration the higher the multiplier (see Table 15). Also, when the multipliers from Table 14 are applied to the environmental exposure scores that result from completing Table 13, the choice of terrestrial values (plants, birds, or mammals) to be used as a multiplier of the soil mobility and persistence score and the choice of aquatic values (microbes, plants, invertebrates, or fish) to be used as a multiplier of the water mobility and persistence score are somewhat arbitrary. The only consideration is that for a given set of terrestrial and aquatic multipliers, the smaller the multiplier used, the smaller the final score for that chemical. If one wishes to present the worst case situation then the largest multiplier should be used. In the following section, in which the scoring system is tested, the mean toxicity multiplier is used. There is no direct multiplier for the air mobility and persistence score; however, the biological effects of a chemical are in many cases the result of atmospheric transport to the terrestrial or aquatic media.

Table 15. Toxicity multipliers of environmental exposure scores

	Terrestrial species (mg/kg)	Aquatic species (mg/liter)	Other[b] (ppm)	Multiplier
Acute[a]	<50	<1	<50 (water) <5 (air) <500 (soil)	3× 3×
	>50 <1,500	>1 <100	>50 <1,000 (water) >5 <100 (air) >500 <10,000 (soil)	2×
	>1,500	>100	>1,000 (water) >100 (air) >10,000 (soil)	1×
Chronic[a]	<10	<0.01	<50 (water) <5 (air) <500 (soil)	3×
	>10 <500	>0.01 <0.5	>50 <1,000 (water) >5 <100 (air) >500 <10,000 (soil)	2×
	>500	>0.5	>1,000 (water) >100 (air) >10,000 (soil)	1×

[a]Values for acute toxicity are either LD_{50}s, LC_{50}s, or GR_{50}s (50% growth reduction), depending on the particular organism. Values for chronic toxicity are concentrations at which an effect is observed. Terrestrial chronic values represent concentrations in diets.

[b]Bacteria and plants.

The terrestrial and aquatic multipliers thus indirectly influence the final toxicity rating of those chemicals whose release is primarily to the atmosphere.

5. TESTING THE MODIFIED SCORING SYSTEM

Adhering to the criteria in Tables 13 and 15. ammonia, linear alkyl sulfonate, 2,4-xylenol, tetraethyllead, quinaldine, and hexachlorocyclopentadiene were scored by using information provided in the chemical dossiers. Table 16 shows the multipliers that were determined, and Table 17 gives the fate and chemistry (environmental exposure) scores for these chemicals. It should be noted that the blanks in Table 16 (indicating no data) are to be expected; they do not serve as indicators of areas that should be examined for testing. The final table (Table 18) shows the integration of the toxicity multipliers from Table 13 with the environmental exposure scores from Table 15 and gives the final scores; the mean terrestrial and aquatic multipliers from Table 16 were applied, respectively, to the soil and to the water scores in Table 17. A ranking of the chemicals in Table 17 (nonintegrated data) according to decreasing environmental exposure scores gives tetraethyllead = hexachlorocyclopentadiene > quinaldine > ammonia > linear alkyl sulfonate > 2,4-xylenol. After integration of the toxicity multiplicity factors (Table 18), the order then becomes hexachlorocyclopentadiene > tetraethyllead > quinaldine > ammonia > 2,4-xylenol > linear alkyl sulfonate. Thus, the order changes, but not significantly. This is especially apparent when the integrated scores of those compounds that decided the changes in the ranking are examined (Table 18); the scores for linear alkyl sulfonate and 2,4-xylenol are very similar, as are the scores for tetraethyllead and hexachlorocyclopentadiene.

6. DISCUSSION AND CONCLUSIONS

Some of the more significant discussions by the workshop participants concerned the following.

1. What is the minimum data set required for scoring as well as the expertise (types of disciplines) necessary for scoring?

Table 16. Toxicity multipliers determined by scoring of test chemicals

Chemical	Terrestrial species				Aquatic species				
	Plants	Birds	Mammals	Mean	Microbes	Plants	Invertebrates	Fish	Mean
Ammonia									
Acute	2×			2×	3×			3×	3×
Chronic			2×						
LAS[a]									
Acute								2×	2×
Chronic							2×		
2,4-Xylenol									
Acute			2×	2×			2×	2×	2×
Chronic									
TEL[b]									
Acute			3×	3×				3×	3×
Chronic									
HCCP[c]									
Acute			3×	3×	3×			3×	3×
Chronic									
Quinaldine									
Acute			2×	2×				2×	2×
Chronic									

[a]LAS = Linear alkyl sulfonate
[b]TEL = Tetraethyllead
[c]HCCP = Hexachlorocyclopentadiene

Table 17. Environmental exposure scores of test chemicals

	Ammonia	Linear alkyl sulfonate	2,4-Xylenol	Tetraethyl-lead	Hexachloro-cyclopentadiene	Quinaldine
Volume	3	3	3	3	2	1
Release	3	3	3	3	2	1
Soil	4	2	2	12	12	2
Air	4	1	1	4	6	2
Water	4	4	4	6	8	12
Bioaccumulation	1	2	1	4	2	2
Total	19	15	14	32	32	20

Table 18. Integration of toxicity multipliers with environmental exposure scores

	Ammonia	Linear alkyl sulfonate	2,4-Xylenol	Tetraethyl-lead	Hexachloro-cyclopentadiene	Quinaldine
Volume	3	3	3	3	2	1
Release	3	3	3	2	1	3
Soil[a]	8	2	4	36	36	4
Air	4	1	1	4	6	2
Water[a]	12	8	8	18	24	24
Bioaccumulation	1	2	1	4	2	2
Total	31	19	20	67	71	36

[a]Terrestrial toxicity multipliers from Table 16 were applied to the soil environmental exposure scores, and aquatic toxicity multipliers were applied to the water scores.

2. Is the scoring exercise a team or an individual effort?
3. How much time is required to effectively score a chemical?
4. What are the drawbacks of the scoring system?

One of the assets of the phase-one scoring system is that a chemical can be scored with only minimal information. Ideally, the completion of all parameters in Tables 13 and 14 is desired; however, a score can be obtained even if some information is not available, as is demonstrated with the six examples in Table 16. Essential to the phase-two (hazard evaluation) scoring system, in addition to biological effects data, is the environmental concentration. The discussion of the scarcity of compounds with measured environmental concentrations and the difficulty in estimating these concentrations emphasized the importance of the phase-one scoring system. The phase-one system can distinguish chemicals that need additional assessment from those that do not; the need for environmental concentrations (measured or estimated) can then be placed as high priority for those compounds selected for further assessment.

The participants thought that a team approach was probably needed to score chemicals because of the breadth of disciplines involved and the necessity of combining separate fate and effect scores. In addition, the lack of pertinent data for many chemicals necessitates sound scientific judgment, and therefore the final score for a chemical should reflect a concensus of scientific opinion. Regardless of how many people are involved in the scoring exercise, the workshop participants felt, approximately 15 minutes would be necessary to effectively score one chemical, although the rate of scoring would be directly related to individual scoring experience.

Some possible drawbacks to the system that were mentioned include (1) the lack of systematic identification of specific data gaps, (2) the lack of identification of potential degradation products or metabolites, and (3) the failure to make judgments concerning the quality of the data. In addition, the use of any systematic chemical screening process involves some degree of error. Professional judgment should be exercised to eliminate as much of the error as possible.

In conclusion, the final scoring system, as presented in Tables 13, 14, and 15 and demonstrated in Tables 16, 17, and 18, is relatively

simple and requires minimal information needs. In addition, the system is recognized as a first cut or first phase approach, the primary purpose of which is to provide a heirarchy of chemicals for consideration for additional assessment. As such it is not a substitute for a hazard evaluation scheme, which is considered a phase-two assessment.

APPENDIX

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16. ABSTRACT

The environmental scoring of chemicals is viewed by the U.S. Environmental Protection Agency as a tool to assist in the ranking or ordering of the universe of chemicals that are under the jurisdiction of the Toxic Substances Control Act. The purpose of scoring is to identify most of the chemicals that have a high probability for requiring review for regulation or testing. This report describes a three-day workshop held in Washington, D.C., August 13-15, 1979, to develop an environmental scoring system. Initial discussions centered on the determination of a safety factor (calculated as the concentration at which an effect is observed divided by environmental concentration) that would allow a numerical score to be assigned to a chemical to reflect its potential hazard. Further discussion, however, indicated that the environmental concentration of a chemical is usually not available and that the estimation of an environmental concentration is not readily accomplished; therefore, a scoring system was developed that does not require environmental concentrations. This system relates environmental exposure to toxicity by using a multiplier (3×, 2×, or 1×) which is assigned on the basis of the concentration at which an effect is observed. The applicability of the scoring system is demonstrated by scoring selected chemicals.

17. KEY WORDS AND DOCUMENT ANALYSIS

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